

Replacement Pages for Claims 1-27

(CLEAN FORM)

1. A method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

representing the instance of symmetry as a list of groups of equivalent atoms and bonds;
and

expressing the instance of chemical structural symmetry in the chemical structure diagram.

2. A method for use in deriving a chemical structure diagram, comprising:

determining, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

C/ applying the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

3. A method for use in deriving a chemical structure diagram, comprising:

determining, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

producing the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram; and

producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

4. A method for use in deriving a chemical structure diagram, comprising:

keeping track of unused display area;

determining a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determining a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

positioning the first and second chemical structure diagrams within the first and second portions, respectively.

5. A system for use in deriving a chemical structure diagram, comprising:

an identifier identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

a representor representing the instance of symmetry as a list of groups of equivalent atoms and bonds; and

an expressor expressing the instance of chemical structural symmetry in the chemical structure diagram.

6. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

an applicator applying the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

7. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram; and

a producer producing the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram, and producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

8. A system for use in deriving a chemical structure diagram, comprising:

a tracker keeping track of available display area;

a determiner determining a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram, the determiner determining a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

a positioner positioning the first and second chemical structure diagrams within the first and second portions, respectively.

9. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

represent the instance of symmetry as a list of groups of equivalent atoms and bonds; and

express the instance of chemical structural symmetry in the chemical structure diagram.

10. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

apply the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

11. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

produce the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram; and

produce a second chemical structure diagram by adding the addition to the first chemical structure diagram.

12. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

keep track of unused display area;

determine a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determine a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

position the first and second chemical structure diagrams within the first and second portions, respectively.

13. The method of claim 1, wherein the instance of chemical structural symmetry is based on rotational symmetry.

14. The method of claim 1, wherein the instance of chemical structural symmetry is based on reflective symmetry.

15. The method of claim 1, wherein the instance of chemical structural symmetry is based on inversive symmetry.

16. The method of claim 1, further comprising:

basing the identification on stereochemistry.

17. The method of claim 1, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

18. The method of claim 1, further comprising:

basing the identification on double bond stereochemistry.

19. The method of claim 1, further comprising:

determining a pivot point for the list.

20. The method of claim 1, further comprising:

determining a graph-theoretic center for the list.

21. The method of claim 1, further comprising:

determining a symmetric order for the instance of chemical structural symmetry.

22. The method of claim 1, further comprising:

determining whether an atom belongs to the determined instance of chemical structural symmetry.

23. The method of claim 1, further comprising:

determining whether a bond belongs to the determined instance of chemical structural symmetry.

24. The method of claim 1, further comprising:

in the event the determined instance of chemical structural symmetry is reflective, selecting a position on an opposite side of a mirror line.

25. The method of claim 1, further comprising:

in the event the determined instance of chemical structural symmetry is rotative, selecting a position based on a pivot point.

26. The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is horizontal.

27. The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is vertical.
